# User's Manual for the USNT Module of the NUFT Code, Version 1.0

**(NP-phase, NC-Component, Thermal)**

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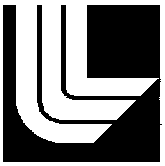

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# 1. Introduction

This manual describes the USNT module of NUFT, which is a model solving the flow and transport equations under non-isothermal conditions of an N-phase system with arbitrary number of components. The balance equations that are solved are given in Appendix C. Local thermodynamic equilibrium is assumed between chemical species using partitioning coefficients. Vapor pressure lowering of components is available as an option.

NUFT (Nonisothermal Unsaturated-Saturated Flow and Transport model) is a suite of multiphase, multicomponent models for numerical solution of non-isothermal flow and transport in porous media with application to subsurface contaminant transport problems. These distinct models are imbedded in a single code in order to utilize a common set of utility routines and input file format.

Currently, the code runs on the Unix and DOS operating systems. Versions have been successfully compiled and tested for IBM-PC compatibles, Cray Unicos, and the following workstations: Sun, Hewlett-Packward, IBM Risc/6000, Silicon Graphics, DEC Alpha. Each set of related models is called a module and has its own user's manual which documents any particular features and input data specific to that module. The NUFT Reference Manual [Nitao, 1993] documents the general numerical algorithms used and gives the documentation of the input to the model common to all or most modules including options not described in the user's manual for each module.

Available modules are:

- `UCSAT` – unconfined and confined saturated flow model
- `US1P` – single phase unsaturated flow (Richard's equation)
- `US1C` – single component contaminant transport
- `USNT` – NP-phase, NC-component with thermal option.

An integrated finite-difference spatial discretization is used to solve the balance equations. The resulting non-linear equation is solved at each time by the Newton-Raphson method. Options for solution of the linear equations at each iteration are direct banded solution and preconditioned conjugate gradient method with various preconditioning schemes.

The model can solve one- , two- , or three-dimensional problems. Future plans include incorporation of capillary hysteresis, non-orthogonal mesh discretization, finite elements, non-linear solid sorption isotherms, and chemical reactions.

The first stage of code verification with one-dimensional problems has been completed (Lee et al., [1993]) and further verification efforts are planned.

The distinct models in the code utilize a common set of utility routines and input file format. The various models are essentially isolated from each other and hence future models can be added without affecting existing models. This also allows for easy maintenance and future enhancements. Global variables in the code are virtually non-existent. The code is written principally in the C language. Input data is in the form of that used by the lisp language. An internal lisp interpreter for the Scheme dialect of lisp is part of the simulator whose purpose is to read the input data file and the internal data files containing default input data values. It also performs data checking.

This manual is self-contained and describes a minimal set of the most commonly used input parameters necessary for the use of this module. The NUFT reference manual (Nitao, [1995])

contains generic input options common to all of most of the modules. It also contains further input options not given in this manual.

**acknowledegments**

The author wishes to thank the management of the Environmental Restoration Division at the Lawrence Livermore National Laboratory (LLNL) for supporting the documentation and verification of the NUFT code. The basic concepts of the code was developed under the funding of the LLNL Institutional Research and Development program.

## 2. How to Install the Model

**Installation onto a Unix System**
The distribution of NUFT for the Unix operating system (Cray Unicos and unix workstations) comes with a C-shell installation script called INSTALL-SCRIPT and a compressed tar file. The name of the compressed tar file is of the form `xxx.tar.Z` where `xxx` are characters referring to the NUFT version number. Copy these two files to any directory (for example, your home directory).

1. Type:

   ```
   csh INSTALL-SCRIPT tar-file
   ```

2. The directory `bin` just below your home directory must be placed as part of your execution path by editing the PATH variable that is usually set in the `.login` file in your home directory, if it is not already there. For example,

   ```
   PATH = .:$HOME/bin:/bin:/usr/bin:/ucb/bin
   ```

3. The installation script and the tar file can be deleted after successful installation. See below for the location of the tar file after installation.

The installation script will create directories `bin` and `NUFT` below your home directory unless they exist already. The installation script creates a directory with the name `xxx` below the NUFT directory derived from the name of the compressed tar file `xxx.tar.Z`. It then copies the compressed tar file and extracts its contents into this directory. It then symbolically links the file `nuft` to the file `nuft-dist` in the installed directory. This is the file that your system executes when you type the `nuft` command which runs the model. NUFT sample input files are also placed into the installed directory.

The script does not remove the directories containing older NUFT versions. The user may delete older versions if they wish. The installation script will give a message indicating whether the installation was successful. After successful installation, the model is ready to run. See the next section in order to run the model.

**Installation for IBM-PC Compatibles under DOS**
The NUFT distribution for IBM-PC Compatibles under DOS comes on a floppy disk with an installation script called `install.bat`.

1. Type:

   ```
   a:\install.bat
   ```

   with the floppy in the `a:` drive.

2. The directory `\nuft` must be placed as part of your execution path by editing the PATH variable that is set in the `autoexec.bat` file in the top directory, if it is not already there. For example,

   ```
   PATH=C:.;C:\;C:\DOS;\nuft
   ```

The installation script will create directories `\nuft` below your home directory unless it exists already. The installation script then creates a directory with the name `xxx` equal to the NUFT

version number and copies the appropriate files there. A file called `nuft.bat` is copied to the `\nuft` directory. This is the file that your system executes when you type the `nuft` command which runs the model. NUFT sample input files are also placed into the installed directory.

The script does not remove the directories containing older NUFT versions. The user may delete older versions if they wish. The installation script will give a message indicating whether the installation was successful. After successful installation, the model is ready to run. See the next section in order to run the model.

## 3. How to Run the Model

Steps to Run the Model:

1. **Install the code.** See the previous section on how to install the code.
2. **Specify the mesh.** The mesh can be created through either of the following methods.
   - Using the `genmsh` option in the input file
   - Using an external program that creates a mesh file (see the NUFT reference manual for description of the mesh file format).

   The first option is recommended for new users.
3. **Create the input data file.** The input file is created using any ascii text editor. An editor such as `vi` or `emacs` which signals matching parentheses is preferable. You will need to read section on the input data syntax to understand the general format of the types of input data that goes into the input file. For first time users it is easiest to edit the preexisting sample input files provided with the code distribution.
4. **Run the model.** Type:

   `nuft` *input-file*

# 4. Input Data Syntax

This section describes the syntax of the input data. The input data file format is in free format, i.e. it does not matter what column the data is in, nor does it matter if the data is continued past the current line or lines.

Input consists of lists of *data blocks, or data units.* Each data unit starts with a left parenthesis and ends with a right parenthesis. A data unit is of the following general form:

(<*name*> <*data*> <*data*> ...)

where

<*name*> refers to the input "variable" that is being set or specified

<*data*> are items which are *real numbers, integer numbers, time real numbers, strings, pattern strings, words,* or other data units, or *list(s)* of data items.

The different data types are defined later in this section.

An alternate form for a data unit is

( \ <*name*> <*data*> <*data*> ... \ <*name*>)

An advantage of this form is that the model can more reliably tell the user the exact location of any unmatching parentheses.

*Example:*

```
(porosity 0.2)
(file-name  "input.data")
(par  0.1 0.3 0.6)
```

This example sets three different variables. It sets the variable `porosity` to the numeric value, `0.2`, the variable `file-name` to the string, `"input.data"`, and the variable `par` to a list of three numeric values, `0.1 0.3 0.6`.

*Example:*

```
(\rocktab  (silt  (porosity 0.3) (Kx 1.e-4)(Ky 1.e-4)(Kz 1.e-4))
           (sand  (porosity 0.2) (Kx 1.e-2)(Ky 0.0)(Kz 0.0))
           (clay  (porosity 0.4) (Kx 1.e-6)(Ky 0.0)(Kz 0.0))
 \rocktab)
```

This example shows how a data unit which sets the variable, `rocktab`, to a list of data units.

**Comment Character:** Semi-colons in the input file serve as comment characters. That is, all characters on a given line after a semicolon are ignored by the program. Using comments is a good way for the user to annotate his input file. Using two semicolons instead of a single one is a good way to make sure that comments standout.

*Example:*

```
(porosity 0.2)  ;; this is how we set the value of porosity to 0.2
```

**Units:** All quantities are in MKS units (i.e. meters, kilogram, seconds). Thus, *hydraulic conductivities* are in meters/second, and *head* is in meters (see Table 4). Unitless quantities such as saturation, porosity, and concentrations are always fractional (i.e. between 0 to 1, inclusive), *not* percentages.

**Legal Data Types:** We now describe the following valid data types.

Table 1 Table of Units used in Input to Models

| | |
|---|---|
| length | *meters (m)* |
| mass | *kilograms (kg)* |
| time† | *seconds (s)* |
| temperature | *centigrade (° C)* |
| area | $m^2$ |
| volume | $m^3$ |
| mass density | $kg/m^3$ |
| molar density | $mole/m^3$ |
| permeability | $m^2$ |
| hydraulic conductivity | $m/s$ |
| flow velocity | $m/s$ |
| force | *Newton* ($Nt=kg\text{-}m/s^2$) |
| pressure | *Pascals* ($Pa=Nt/m^2$) |
| head | $m$ |
| energy | *Joule* ($J=Nt\text{-}m$) |
| specific energy | $J/kg$ |
| mass flux | $kg/s$ |
| molar flux | $mole/s$ |
| volumetric flux | $m^3/s$ |
| energy flux | *Watts* ($W=J/s$) |
| thermal conductivity | $W\text{-}m/\,°C$ |
| dynamic viscosity | $Nt\text{-}s/m^2=kg/m\text{-}s=10^3$ *centipoise* |
| molecular diffusivity | $m^2/s$ |

†model can accept other time units using unit designators

1. A *string* is any sequence of visible characters delimited by double quotes "", for example,

   ```
   "hello there"
   " run3-B (test#2) "
   ```

   Note that spaces and parentheses are allowed in a string.

2. An *integer number*, for example, `11`.

3. A *real number* that is fixed or floating point. For example `1.23, -4.5e7, or 900.2E7`. Note that **D or d exponents in the manner of FORTRAN are not allowed !**

4. A *time number* which is a real number but with with the following unit designators as the last letter in order to denote units of time. As you may have guessed, this type of number is used whenever we want to specify a time.

   | | |
   |---|---|
   | s | seconds |
   | m | minutes |
   | h | hours |
   | d | days |
   | M | months |
   | y | years |

   If no unit designator is present, then seconds is assumed.

   *Examples:*

   | | |
   |---|---|
   | 20.0 | 20 seconds |
   | 23.1s | 23.1 seconds |
   | 45e4M | 45e4 months |

   There must be no spaces between the number and the unit designator.

5. A *word* is a sequence of non-blank visible characters. A word can be a variable or may be used in the same way as a string except that it can not have internal blanks. The model treats the words and strings as being distinct data types; the correct one as specified in the documentation is required.

6. A *pattern string* is a special type of a string with the two unix shell type "wild" characters

   `*` and `?`

   so that a pattern string can represent an entire class of strings that matches the string pattern. The character `*` in a pattern matches any sequence of characters. Hence, the pattern `"*"` matches all strings. The character `?` in a pattern matches any single character. Hence, the patter `"?"` matches all strings with exactly one character.
   *Other Examples:*

   1. The pattern `"ex*"` matches all strings that begin with the characters `"ex"`.
   2. The pattern `"ex*b2*z"` matches all strings that begin with `"ex"`, followed by any number (including zero) of strings which are then followed by the string `"b2"`, and which end with the string `"z"`.
   3. The pattern `"r2?xay"` matches all strings that begin with `"r2"` followed by a single character, and then followed by the characters `"xay"`.

**Include statement:**

The include statement is of the form

`(include "<`*file-name*`>")`

It is used to place the contents of the file with the name, "<*file-name*>", into the input file. The file must lie in the working directory under which NUFT is being run. It can only be used to replace a complete list, i.e. must be either a collection of data which is delimited by a closed sets of parentheses or a single data item such as a number or string. For example, suppose the file "data1.inc"contains

```
(field (format list) (range "*") (variables S1)(file-ext ".S1")
       (outtimes 0 70m 102m 222m 287m 342m 23h)
)
```

and the file "data2.inc"contains the single entry

```
200m
```

with the file "data3.inc"containing the string

```
".S1"
```

Then, the following input data

```
(output
     (include " data1.inc")
     (forcetimes (outtimes (include " data2.inc" 201m))
)
```

will be interpreted by the model as begin equivalent to

```
(output
     (field (format list) (range "*") (variables S1)(file-ext ".S1")
            (outtimes 0 70m 102m 222m 287m 342m 23h)
     )
     (forcetimes (outtimes 200m 201m))
     (file-ext ".S1")
)
```

The following is an example of an error. Suppose the file "file.inc"contains the following

```
(outtimes 0 70m 102m 222m
```

and the input file as the data item

```
(output
     (field (format list) (range "*") (variables S1)(file-ext ".S1")
            (include " file.inc")  287m 342m 23h)
     )
     (forcetimes (outtimes 200m 201m))
     (file-ext ".S1")
)
```

This is an error because only complete lists or a single entry can be included (not to mention the fact that the parentheses will not match in the input file).

**Include package statement:**

The include package statement is of the form

`(include-pkg "<`*file-name*`>")`

This statment is identical to the `include` statement except that it includes a file from the subdirectory which contains the NUFT executable instead from the current working directory. The main purpose is to include a 'package' of pre-defined input parameters which comes with the NUFT software distribution.

**Macro commands:**

Macro commands start with the character '#'. There are three commands available: `#define`, `#ifdef`, and `#ifndef`. The following command defines a macro variable,
`(#define <`*variable*`>)`
Currently, a variable cannot be defined to be any particular value, but it is used in conjunction with the other macro commands. The statements within
`(#ifdef <`*variable*`> .... )`
will be placed as part of the input stream if <*variable*> is defined by the `#define` command; whereas, the statements within
`(#ifndef <`*variable*`> .... )` will not be placed as input if <*variable*> is not defined. The `#define` statements must be in the same parenthesis level as, for example, `bctab`, `genmsh`, etc. The `#ifdef` and `#ifndef` commands can be placed anywhere, except that the body of statements in the conditional commands must be complete lists, i.e. parentheses match inside the macro command. Currently, the macro commands only work inside an input set for a module or inside `common`.

## 5. Input Format

Before going further the user should read the section on the input data syntax.

**Form of Input Data**

```
(usnt
     (init-eqts ...)  ;; set names of components and phases
     (title ...)      ;; run title
     (output-prefix ...)  ;; prefix of all output files
     (time ...)       ;; initial time
     (tstop ... )     ;; ending time
     (dt ...)         ;; initial time step size
     (dtmax ...)      ;; maximum time step
     (stepmax ...)    ;; maximum no. of time steps
     (tolerdt ...)    ;; absolute time step control
     (reltolerdt ...) ;; relative time step control
     (tolerconv ...)  ;; absolute Newton-Raphson convergence criteria
     (reltolerconv ...)  ;; relative Newton-Raphson convergence criteria
     (genmsh ...)        ;; mesh specification
     (read-restart ...)  ;; read initial data from restart file
     (state ...)      ;; set initial conditions
     (compprop ...)   ;; component dependent property values
     (phaseprop ...)  ;; phase dependent property values
     (generic ...)    ;; generic property values
     (rocktab ...)    ;; porous medium properties
     (output...)      ;; output specification (optional)
     (srctab ...)     ;; source term tables (optional)
     (bctab ...)      ;; boundary condition tables (optional)
)
```

The '...' denote data which will be explained later. All input past a semicolon on a given line is treated as comments. The above data units can occur in any order except for the word `usnt` which must come first. Either `state` or `read-restart` must be present, but not both. The items `(output ...)`, `(srctab ...)`, and `(bctab ...)` are optional; the rest are required. There are other optional data items not shown above that are described in the NUFT Reference Manual (Nitao, [1995]).

## 6. Input Data Documentation

In this section we describe all of the basic input data needed to run the model. Some less widely used options are documented in the *NUFT Reference Manual.*

**Specify component and phase names.**

```
(init-eqts
     (components  <comp> <comp> ...)
     (phases <phase> <phase> ...)
     (wetting-phase <wetting-phase>)
     (<thermal-option>)
)
```

Set names of phases and components. Also, specifies whether the model is isothermal or thermal and sets the wetting phase.

*<comp>* *word*

Name of component. NUFT solves the coupled set of balance equations for each component. The components can be in any order. The ordering can impact some of the other input parameters which refers to components by this tacit ordering. The component `energy` should not be specified here even though the model internally uses this component name when the model is thermal (i.e. *<thermal-option>* is set to `thermal`). Although one may give the components any name, some components have significance. When using equation of state options specific to an "air" (pseudo) component or to a "water" component, one must use the appropriate component names, `air` or `water`, respectively.

*<phase>* *word*

Name of phase. Currently, the model require one of the phases to be a gas phase, so that `gas` should be one of the phase names. An aqueous phase should be called either `liquid` or `aqueous`.

*<wetting-phase>* *word*

The name of the fluid phase which is in contact with the solid, withing which partitioning of a component occurs with the solid due to sorption onto the solid. The $Kd$ values are defined with respect to this partitioning.

*<thermal-option>* *word*

NUFT will solve the balance equation for energy in order to calculate the temperature if this parameter is set to `thermal`. If set to `isothermal`, the energy balance equation is not solved. For the thermal option, the initial temperature is set by `state` data item. For isothermal models, the initial temperatures are set in the `generic` data item.

*Example:*

```
(init-eqts
     (components  water air TCE)
     (phases aqueous gas NAPL)
     (wetting-phase liquid)
     (isothermal)
)
```

**Title and output file prefix.**

`(title "<`*run-title*`>")`

"<*run-title*>" *string*

string containing the title of the run. The string will be placed in the header of output files.

`(output-prefix "<`*prefix*`>")`

"<*prefix*>" *string*

Optional. All output file names will have this prefix. All output files will have this prefix unless set to otherwise. The main output file has this prefix with suffix "`.out`". *Example:* setting

```
(output-prefix "runA")
```

will set the main output file name to be called "`runA.out`". Other auxillary output files can be created from separate suffixes set by the `file-ext` parameter in the various output options possible using the `output` data unit. Default is to use the prefix of the input file name. For example if the input file is called `runA.3.in`, then the output files have the prefix `runA.3`, such as `runA.3.out`.

**Time step control.**

`(time` *<start-time>*`)`

*<start-time>* *t-real*

initial starting time of run. For restarts, this time is not needed if `restart` is set, in which case the initial time will be set to the time read in through the restart file. If `time` appears, this overwrites the time read in.

`(tstop` *<stop-time>*`)`

*<stop-time>* *t-real*

run will stop when it reaches this time.

`(dt` *<initial-time-step>*`)`

*<initial-time-step>* *t-real*

initial time step size.

`(dtmax` *<max-step-size>*`)`

*<max-step-size>* *t-real*

maximum time step size.

`(stepmax` *<max-steps>*`)`

*<max-steps>* *integer*

maximum number of time steps; run will stop if this will be exceeded.

**Time step control.**

`(tolerdt (P` *<tolerdt-P>*`) (S` *<tolerdt-S>*`) (C` *<tolerdt-C>*`)`
`(T` *<tolerdt-T>*`)` *present only for thermal models*
`)`

Set absolute tolerances for time step control.

*<tolerdt-P>* *real*
*<tolerdt-S>* *<tolerdt-S>...* *reals*
*<tolerdt-C>* *<tolerdt-C>...* *reals*
*<tolerdt-T>* *real*

The model will control time step such that the magnitude of changes in the primary variables: gas pressure `P` (Pa), saturations `S` (fraction), mole fraction concentrations `C` (mole fraction), and temperature `T` (deg. C) from one time step to the next does not exceed the specified values. The tolerance for the saturation of a particular phase or the concentration of a particular component can also be specified and overwrites the general value set by `S` or `C`. For example,

```
(tolerdt (P 1e3) (S 0.25) (S.liquid 0.1) (C 0.01) (C.TCE 1e-7))
```

sets the tolerance for the liquid saturation to 0.1 and 0.25 for all other phases and the tolerance for concentration of the component TCE to 1e-7 and all other concentrations to 0.01. As a rule of thumb the tolerances should be about one to two orders of magnitude larger than the desired accuracy of the primary variable. Recommended tolerances for pressure is 0.2 times the maximum initial pressure. Tolerance for saturations is 0.25, concentrations 0.2 and temperature 15 degrees. Tolerances for some concentrations such as for a low level contaminant may have to be much lower.

`(reltolerdt (P` *<reltolerdt-P>*`) (S` *<reltolerdt-S>*`) (C` *<reltolerdt-C>*`)`
`(T` *<reltolerdt-T>* *present only for thermal models*
`)`

Set relative tolerances for time step control. The model calculates a time step based on the absolute tolerance set in `tolerdt` and another time step based on relative tolerances set in `reltolerdt` and uses the larger of the two.

*<reltolerdt-P>* *real*
*<reltolerdt-S>* *<reltolerdt-S>...* *reals*
*<reltolerdt-C>* *<reltolerdt-C>...* *reals*
*<reltolerdt-T>* *real*

The model will also control time step such that the relative magnitude of changes in the primary variables: gas pressure `P`, saturations `S`, and concentrations `C` from one time step to the next does not exceed the specified values. For each primary variable the model calculates the largest magnitude over all the elements in the entire problem domain and then multiplies by the specified relative tolerance to get a maximum change. Recommended

tolerance for pressure is 0.2, saturation 0.0, concentration 0.2, temperature 0.0. Note that a zero tolerance causes the model to ignore relative tolerances and use the absolute tolerance. In the same way as for the `tolerdt` statement, tolerances for saturations of specific phases and concentrations of specific components can be set.

**Newton-Raphson convergence tolerances.**

`(tolerconv (P` *<tolerconv-P>*`) (S` *<tolerconv-S>*`) (C` *<tolerconv-C>*`)`
`(T` *<tolerconv-T>*`)` *present only for thermal models*
`)`

Sets tolerances for Newton-Raphson iteration convergence criteria. The model checks for convergence using both the `tolerconv` and `reltolerconv` parameters. Convergence is assumed if either one of the criteria is true for each primary variable.

*<tolerconv-P>* *real*
*<tolerconv-S>...* *reals*
*<tolerconv-C>...* *reals*
*<tolerconv-T>* *real*

Absolute criteria for convergence of the Newton-Raphson iterations for solution of the non-linear, implicit-in-time, discretized balance equations is acheived if the magnitude of the changes in the primary variables: gas pressure `P` (Pa), saturations `S` (fraction), concentrations `C` (mole fraction), and temperature `T` (deg. C) from one iteration to the next is less than or equal to these values. Recommended tolerance for pressure is 0.0001 times the maximum initial pressure, for saturation is 0.001, for concentration is 0.0001, and temperature 0.01. The tolerance for a dilute component, such as a contaminant, should have a much lower tolerance equal to 0.01 times the the level of desired absolute accuracy. In the same way as for the `tolerdt` statement, tolerances for saturations of specific phases and concentrations of specific components can be set.

`(reltolerconv (P` *<reltolerconv-P>*`) (S` *<reltolerconv-S>*`) (C` *<reltolerconv-C>*`)`
`(T` *<reltolerconv-T>*`)` *present only for thermal models*
`)`

Sets relative tolerances for Newton-Raphson iteration convergence criteria. The model checks for convergence using both the `tolerconv` and `reltolerconv` parameters. Convergence is assumed if either one of the criteria is true for each primary variable.

*<reltolerconv-P>* *real*
*<reltolerconv-S>* *<reltolerconv-S>...* *reals*
*<reltolerconv-C>* *<reltolerconv-C>...* *reals*
*<reltolerconv-T>* *real*

Criteria for Newton-Raphson convergence based on the maximum relative magnitude of changes in the respective primary variables. Recommended values are 0.001 for pressure, 0.01 for saturation, 0.001 for concentrations, and 0.001 for temperature. In the same way as for the `tolerdt` statement, tolerances for saturations of specific phases and concentrations of specific components can be set.

**Generate mesh.**

```
(genmsh
     (coord  <mesh-type>)
     (down <Vx> <Vy> <Vz>)
     (dx <dx-1> <dx-2> ...)
     (dy <dy-1> <dy-2> ...)
     (dz <dz-1> <dz-2> ...)
     (mat
          (<el-name-prefix><mat-type>
               <i0><i1> <j0><j1> <k0><k1>)
                    ...
          (<el-name-prefix><mat-type>
               <i0><i1> <j0><j1> <k0><k>)
     )
     (anisotropic)
     (wrap-around)   optional
)
```

specifies the mesh geometry, element material types and names.

*<mesh-type>* *word*

specifies the type of mesh that will be generated. Valid options:

| | |
|---|---|
| `rect` | rectangular mesh |
| `cylind` | cylindrical mesh |

Let the three coordinates of our mesh system be $x$, $y$, and $z$. If the mesh type is `rect`, then $x$, $y$, and $z$ are along the coordinate axes of a rectangular system. If mesh type is `cylind`, then the first coordinate $x$ is the radial distance $r$, the second coordinate $y$ is angle $\theta$, and the third coodinate $z$ is the longitudinal axis.

*<Vx> <Vy> <Vz>* *reals*

are the components of the vector pointing downward in the direction of the gravity vector. The program will internally normalize the vector to unity. Setting the components to all zero will turn off gravity in the model. The vector is always with respect to a rectangular coordinate system $(X, Y, Z)$. For a rectangular mesh, the coordinate system coincides with the rectangular coordinate system $(x, y, z)$ of the mesh. If the mesh is cylindrical, the vector is with respect to a coordinate system $(X, Y, Z)$ where $X$ is the axis defined by $\theta = 0, z = 0$; $Y$ is the axis defined by $\theta = 90°, z = 0$, and the axis $Z$ is defined by $r = 0$.

*<dx-1> <dx-2> ...* *reals*

are the subdivisions of the mesh in the direction of the first coordinate $x$. For a rectangular mesh, the subdivisions are in the increasing $x$ direction of the rectangular coordinate system of the mesh. For a cylindrical mesh, the subdivisions are in the increasing $r$ direction. Numbers that are repeated can be abbreviated; for example, `3*5.0` would stand for three repeats of the numeral `5`, that is, `5.0 5.0 5.0`.

*<dy-1> <dy-2> ...* *reals*

are the subdivisions of the mesh in the direction of the first coordinate $x$. For a rectangular mesh, the subdivisions are in the increasing $y$ direction. For a cylindrical mesh, these parameters set the subdivisions in the increasing $\theta$ direction. Angular units are in *degrees*. The cylindrical mesh wraps completely around the $\theta$ direction only for the case of a single angular subdivision whose value is equal to *dy-1* = 360°).

*<dz-1> <dz-2> ...* *reals*

are the subdivisions of the mesh in the increasing $z$ direction for either a rectangular or cylindrical mesh system.

*<el-name-prefix>* *word*

prefix of element name. Each element in the specified $i, j, k$ index range will a name comprised of this prefix and a number associated with it as the suffix (see the explanation of index ranges below for examples). This prefix can be used to specify a range of elements in the `state`, `output`, and other input parameters. The element names will be of the form *<el-name-prefix>*`#`*<i>*`:`*<j>*`:`*<k>* where *<i>*,*<j>*,*<k>* denote the $i$, $j$, and $k$ indices.

*<mat-type>* *word*

material type. Each element in the specified $i, j, k$ range will have this material type (see the explanation of index ranges below for examples). Each material type must have a corresponding entry in the material type table in `rocktab`. An exception are material types that are pre-defined in the model. At this time, the only pre-defined material type is `NULL` which completely removes the respective element or elements from the model. An equivalent method of removing elements is the `null-blocks` option describedin the NUFT Reference Manual. Material types that are of the following form denote specific 'auxillary' elements used for boundary conditions,

`BC.1.xxx` element for b.c. of first type,
`BC.2.xxx` element for b.c. of second type,
`BC.3.xxx` element for b.c. of third type.

An element for first and third type boundary conditions will have zero flow connection from the element centroid to the boundary of any neighboring non-auxillary elements. An element for a second type boundary condition will have flow connection set to unity so that the reciprocal of the permeability or hydraulic conductivity will be the resistance, and the volume of the element is set to the average volume of neighboring non-auxillary elements.

*<i0> <i1> <j0> <j1> <k0> <k1>* *integers*

specifies a range of elements using the $i, j, k$ indices of the element in the direction of the $x, y, z$ directions. Used to specify the range of elements for setting element name prefixes *<el-name-prefix>* and the material types *<mat-type>*. **A specification record of the form,**

(*<el-name-prefix><mat-type><i0><i1><j0><j1><k0><k1>*)

**will overwrite the effect of any previous records (see example below).** In this way, one can specify non-rectangular regions to have the same element prefix or material type.
The $i, j, k$ indices are consistent with the `dx`, `dy`, and `dz` parameters. That is,

the `dx` parameter specifies the $x$ dimension of the elements for $(i = 1, 2, \ldots)$, in that order. Similarly, `dy` specifies the $y$ dimensions of the elements for $(j = 1, 2, \ldots)$, and `dz` specifies the $z$ dimensions for $(k = 1, 2, \ldots)$.
*Example:*

```
(e silt 2 4 3 10 1 8)
```

This example specifies that the elements in the index range ($i = 2$ *to* 4), ($j = 3$ *to* 10), and ($k = 1$ *to* 8) will have element names `e1, e2,` ... and will be of material type `silt`.
*Example:*
consider a mesh with 4 elements in the $i$ direction, 3 elements in the $j$ direction, and 5 elements in the $k$ direction,

```
(mat
     (s  silt  1 4  1 3  1 5)   ;; first set all elements
                                ;; to silt
     (c  clay  1 4  1 3  2 2)   ;; make layer k=2 into clay
     (w  well  2 2  3 3  2 2)   ;; make i=2,j=2, k=2 into
                                ;; well element
     (aquif silt 1 4  1 3  5 5) ;; call lowest layer by
                                ;; different prefix
 )
```

The symbols `nx`, `ny`, and `nz` can be used anywhere in place of a number where an index is required. The model interprets these to mean the number of subdivisions in the x, y, and z directions, respectively.

`(anisotropic)`

this parameter is optional. (The older form of the parameter `isot-dir` can also be used instead.) Affects the choice of the permeability (or hydraulic conductivity) parameter. See the documentation of the parameters `Kx`, `Ky`, and `Kz` below. This parameter should not be present for models where isotropic permeability (or hydraulic conductivity) is desired unless the three permeability parameters for each material type are equal.

`(wrap-around)`

if present, model wrap the grid around in the angular direction. I.e. for each element at $j = 1$ connect to the corresponding adjacent element at $j = ny$ where $ny$ is the number of elements in the $j$ direction. Default is no wrap-around.

**Specify initial conditions.**

```
(state
     (<state-var-name>  <method>  <data>)
        ...
     (<state-var-name>  <method>  <data>)
)
```

Set initial state variables.

Let NP be the number of phases in `init-eqts`, let NC the number of components, and let NPNZ be the number of phases with nonzero saturation. The state variables which must be initialized at each element are: gas pressure, first NP-1 nonzero saturations in order of the phases as they appear in `init-eqts`, concentrations of last NC-NPNZ components (in the order as they appear in `init-eqts`) in the phase which is the first one with nonzero saturation in the order given in `init-eqt`. For thermal models, the temperature must also be initialized. The NP-th saturation is internally computed from the constraint that the sum of the saturations is unity. The concentrations of the first NPNZ components is calculated from conditions for local thermodynamic equilibrium. Note that, not counting the saturation which are zero, there are NC primary variables for isothermal models and NC+1 primary variables for thermal models. This is the same number as the number of balance equations for each component and for energy.
For example, consider a system with two phases, liquid and gas, and three components, air, water and a contaminant,

```
(init-eqts
    (phases liquid gas)
    (components air water contam)
    (wetting-phase liquid)
    (isothermal)
)
```

If the liquid and gas saturations are both non-zero then the primary variables are gas pressure, liquid saturation, and concentration of the contaminant in the liquid phase. If the liquid saturation is zero then the primary variables are gas pressure and concentration of water concentration of contaminant, both in the gas phase.

*<state-var-name>* *word*

The valid primary, or state, variable names are

| | |
|---|---|
| `P` | absolute gas pressure (Pa) |
| `S.`*<phase>* | saturation (fraction) |
| `C.`*<comp>* | contaminant concentration (mole fraction) |
| `T` | temperature, if model is thermal (Centigrade) |

where *<phase>* is the name of a phase which is one of the first NP-1 phases set in `init-eqts`, NP being the number of phases. The model internally calculates the saturation of the NP-th phase from the constraint that the saturations must sum to unity. *<comp>* is a name of a component set in `init-eqts` (excludes the `energy` "component"). Only the last NC-NPNZ concentrations in the order of the components occuring in `init-eqt` are used by the model. The other concentrations should be set to a negative number. In this way the model can check to see if the concentration is really needed in that if it is needed and it is negative, it will let the user know by giving a fatal error message in the main output file. If a concentration is non-negative but is not necessary, a warning message is flashed to output.

If a saturation is initialized to a value greater than the maximum liquid saturation (as set in `rocktab`), then it is reset by the model to that value. If the saturation is set to a value less than zero, it is reset to zero.

*<method>* *word*

chooses the format by which the initial conditions will be set. See below for valid formats.

*<data>*

Valid data formats are:

`by-key` ("*<elem-range>*"*<value>*)
initialize elements that are within the element range.
"*<elem-range>*" *pattern string* elements whose names match this pattern will be set to the specified value. *<value>* *real*
elements in the specified range will have this value for the specified primary variable.

Example:
`(C by-key ("el*") 0.1)` sets the initial value of the variable, `C`, to 0.1 for all elements whose names begin with the characters `el`.

`by-set` *<vector>*

initialize all components of the vector holding the . Ordering of vector is relative to internal ordering done by code. Used for transfering values from an output from a previous run.
*<vector>* = [#*<n>* *<v0>* *<v1>* ...]
where *<n>* is no. of elements (the #*<n>* field is optional) and *<v0>* *<v1>* ...are of type *real* and are the initial values. Here, [and ]are actual characters and do not represent delimiters of optional parameters
*Example:*

```
(Sl by-set [#3 3.  4.  1.])
```

Sets the variable `Sl` to the values 3., 4., 1. for element numbers 1,2, and 3, respectively.

`by-xtable` *<table>* or
`by-xtable` `(range "`*<elem-range>*`")` *<table>*

sets initial condition by interpolating from a table of values specified at given values of the $x$ coordinate.

"*<elem-range>*" is an optional range of elements whose state variable will be set. Default is all elements.
*<table>* is a table of values with respect to the appropriate x,y, or z coordinate. The table is of the form:
(*<x0>* *<val0>* *<x1>* *<val1>* ...) or *<x0>* *<val0>* *<x1>* *<val1>* ... where *<x0>* *<x1>* ...are the values of the $x$ coordinate and *<val0>* *<val1>* ...are the values of the primary variable that is being initialized. Values are calculated

using linear interpolation based on the coordinates of the element centroids. Centroid coordinates are derived from the subdivisions specified in `dx`, `dy`, and `dz` parameters. The coordinates of the edges of the model start at zero, so that, the $x$ coordinate for the element centroids for $i = 1$ are $x =$<*dx-1*>/2, those for $i = 2$ are $x =$<*dx-1*> + <*dx-2*>/2 and so on. The $y$ coordinate for the element centroids for $j = 1$ are $y =$<*dy-1*>/2, those for $j = 2$ are $y =$<*dy-1*> + <*dy-2*>/2 and so on, and, similarly, for the $z$ coordinates.

`by-ytable`

sets initial condition through a table of values versus the $y$ coordinate.

`by-ztable`

sets initial condition through a table of values versus the $z$ coordinate.

A state variable can appear more than once to overwrite values set by previous specification records. It is often convenient to set the values for all elements by `by-ztable` or `by-set` and then modify values for specific elements using `by-key)`. For example,

```
(state
     (C by-ztable  (0.0 0.0   1. 2.  10 2.))
     (C by-key  ("abc*" 0.0))
     (C by-key  ("*D*" 1.0))
)
```

The first record initializes the variable `C` by a table given with respect to the $z$ coordinate of the element centroid. The second record overwrites the value of `C` to 0.0 for those elements whose names (set by the `genmsh` input parameters) begin with the characters `abc`. The third record overwrites the value to 1.0 for those elements whose name contains the letter `D`.

NOTES:

1. A state variable can appear more than once to overwrite values set by previous specifications; for example, values for all elements can be set by "`by-xtable`" or "`by-set`" and then "touched up" using "`by-key)`".
2. The program will terminate if a primary variable has not been set for all of the elements.

*Example:*

Consider a system with two phases and three components as specified by

```
(init-eqts
    (phases liquid gas)
    (components air water contam)
    (wetting-phase liquid)
    (isothermal)
 )
```

Example of how initial conditions can then specified is given by the following:

```
(state
     (C.contam by-ztable
```

```
                ;; height
                ;; above
                ;; WT     C.contam
                   (0.0   0.0
                    0.2   0.001
                    0.8   0.01
                    1.0   0.01
                   10.0   0.0
                  )
        )
        (C.water ("*" -1.0) ("atm*" 0.02))

        (S.liquid by-ztable
                ;; height
                ;; above
                ;; WT     S.liquid
                   (0.0   1.0
                    0.2   0.9
                    0.8   0.5
                    1.0   0.4
                   10.0   0.3
                  )
        )
        (S.liquid by-key ("bc*" 1.0))
        (S.liquid by-key ("atm*" 0.0))
        (P by-key  ("*" 1.e5))
)
```

In this example, the concentrations `C.contam` are `S.liquid` are first initialized by interpolating from tables specifying values vs. height above the water table. Then, liquid saturation is for elements with names starting with the characters `"bc"` is set to unity and those with leading characters `"atm"` is set to zero. The water component concentration is required for the elements with zero liquid saturation and is set to 0.02. All other elements are set to a negative number to let the model check whether we have overlooked anything if they are needed. The pressure of all of the elements is initialized to 1.e5 Pa.

**Material properties.**

```
(rocktab

     (<rock-type name>

          (porosity <porosity>)

          (Kd (<comp> <Kd>) (<comp> <Kd>) ...)

          (tort (<phase> <tort-parameters>)
                ...
                (<phase> <tort-parameters>))

          (Kx <perm-x>) (Ky <perm-y>) (Kz <perm-z>)

          (pc (<phase> <pc-parameters>)
              ...
              (<phase> <pc-parameters>))

          (kr (<phase> <kr-parameters>)
              ...
              (<phase> <kr-parameters>))

       following are needed only if model is non-isothermal

          (Cp <Cp>)

          (solid-density <solid-density>)

          (tcond <tcond-option>
               (solid <tcond-solid>)
               (<phase> <tcond-sat>)...(<phase> <tcond-sat>))

          (KdFactor (<comp> <KdFactor-parameters>)
                    ...
                    (<comp> <KdFactor-parameters>))

     )

     ...

     (<rock-type name>

          ...

     )

)
```

Set material properties for flow model. Each element has a porous medium material property type specified in the `genmsh` data item. The model references this type when it calculates various contitutive properties which depend on the material type such as char-

acteristic curves, porosity, etc.

*<rock-type-name>* *word*

Name of the material. Can be any name.

*<porosity>* *real*

The fractional porosity of the material. Needs to be a number greater than zero, otherwise the system will of equations solved by the model becomes mathematically singular.

*<Kd>* *real*

Dimensionless solid sorption coefficient of the component defined as the quantity $\rho_B k_d/\phi$ where $\rho_B$ is bulk dry density (g/ml), $k_d$ is the standard solid sorption coefficient (ml/g), and $\phi$ is porosity. Given a soil sample, $k_d = \omega_s/C_\alpha$ where $\omega_s$ is $\mu$g of component sorbed on the solid divided by the mass of the solid in the sample in units of grams and $C_\alpha$ is $\mu$g of component dissolved in the wetting phase $\alpha$ divided by the volume of the phase in ml. If $\rho_B$ is given in units of g/ml then $\rho_B k_d = C_s/C_\alpha$ where $C_s$ is $\mu$g of sorbed component divided by the bulk volume of the sample in ml. It is well known that $R = 1 + \rho_B k_d/\phi$ where $R$ is the "retardation factor" for flow when the porous medium is saturated by the wetting fluid. Thus, $\rho_B k_d/\phi = R - 1$.

*<tort-parameters>* *real*

Parameters for calculating tortuosity factor $\tau$ for *<phase>* which used is the factor multiplying the free molecular diffusion coefficient in calculating the diffusive flux of a component. The diffusion flux is given by

$$q_\alpha^\gamma = -\rho_\alpha \phi S_\alpha \tau_\alpha \mathcal{D}_\alpha^\gamma \nabla \omega_\alpha^\gamma$$

| | |
|---|---|
| $q_\alpha^\gamma$ | mass flux |
| $\rho_\alpha$ | mass density of $\alpha$ phase |
| $S_\alpha$ | saturation |
| $\mathcal{D}_\alpha^\gamma$ | free diffusion coefficient for $\gamma$ component |
| $\omega_\alpha^\gamma$ | mass fraction |

Following are valid options:

*<real-value>*

Constant value. Usually greater than or equal to zero and less than or equal to one. Setting to zero will turn off diffusion of all components in *<phase>*.

`Millington`

Millington formulation given by

$$\tau_\alpha = S_\alpha^{7/3} \phi^{1/3}.$$

<*perm-x*> *real*
<*perm-y*> *real*
<*perm-z*> *real*

Intrinsic absolute permeability ($m^2$) of the material. The model normally will use only the value of <*perm-x*>. The other two values are ignored although they must be present and can be set to zero. However, if the parameter `anisotropic` or `isot-dir` is present in data unit `genmsh`, then the value of <*perm-x*> will be used for flow in the first coordinate direction (for example, $x$-axis direction for rectangular coordinates and $r$-axis for cylindrical), <*perm-y*> will be used for the second coordinate direction ($y$ or $\theta$), and <*perm-z*> for the third coordinate direction ($z$).

<*pc-parameters*> *list of data units*

Parameters for calculating the pressure difference ("capillary pressure") between the gas phase and a nongas phase

$$p_c = p_g - p_\alpha\,, \qquad \alpha \neq g$$

as a function of the saturations. An entry for `pc.`<*phase*> is needed only for <*phase*> over all nongas phases. Valid options are

<*real*>

Constant value. A zero value is used to simulate an element that is in a non-porous medium where the phase pressures are equal.

`pcVanGen (m` <*m*>`) (alpha` <*alpha*>`) (Sj` <*Sj*>`) (Sa` <*Sa*>`) (Sr` <*Sr*>`) (Smax` <*Smax*>`)`

Van Genuchten formulation.

<*m*>

Parameter (unitless).

<*alpha*>

Parameter (1/Pa).

<*Sj*>

Optional. Transition saturation below which a linear curve is used. The default is $Sj = Sr + 0.05 * (Smax - Sr)$.

<*Sa*>

*(optional)* A linear function will be used for liquid saturation greater than <*Sa*> and less than or equal to the maximum saturation to avoid the infinite slope at maximum saturation. Default is 0.999 times the maximum saturation.

<*Sr*>

Residual saturation.

<*Smax*>

Optional maximum saturation. Default is unity.

*<kr-parameters>* *list of data units*

Name of the liquid relative permeability function vs. saturation function and its associated parameters. Valid options are:

*<real>*

Constant value. Usually between zero and one, inclusive. A zero value can be used to shut off advective flow of the phase exiting an element since the model uses upstream weighting of the mobility factor $k_r/\mu$ as the default.

`krlVanGen` (`m` *<m>*) (`Sa` *<Sa>*)
`krgVanGen` (`m` *<m>*) (`Sa` *<Sa>*)
`krfVanGen` (`m` *<m>*) (`Sa` *<Sa>*)

Van Genuchten formulation for aqueous, gas, and free hydrocarbon phase, respectively.

*<m>*

Parameter (unitless).

*<Sa>*

*(optional)* If (`Sa` *<Sa>*) is present, then a linear function will be used for liquid saturation greater than *<Sa>* and less than or equal to the maximum liquid saturation (= one minus the residual gas saturation) to avoid the infinite slope at maximum saturation. Default value is 0.999 times the maximum saturation.

`krgVanGenMinus`

Calculates gas relative permeability as one minus the liquid permeability. Used only for two-phase gas-liquid systems.

`krlLinear`
`krgLinear`
`krfLinear`

Linear relative permeability function for aqueous, gas, and free hydrocarbon phase, respectively,

$$k_r = (S - S_r)/(S_{max} - S_r).$$

*<Cp>* *real*

Specific heat of the solid (J/kg).

*<solid-density>* *real*

Solid grain density (kg/m$^3$).

*<tcond-solid>* *real*

Bulk thermal conductivity of the porous medium (J/s-C) when there is no fluid at all in the pore space.

*<tcond-sat>* *real*

Bulk thermal conductivity of the porous medium (J/s-C) when the phase denoted by *<phase>* completely fills the pore space.

*<tcond-option>* word

Options for calculating saturation dependent bulk thermal conductivity:

`tcondLin`

The total bulk conductivity is calculated using a linear weighting of saturations

$$k^{bulk} = k^{dry} + \sum_{\alpha=1}^{NP} S_\alpha k_\alpha^{sat}.$$

`tcondLin`

A square root weighting is used,

$$k^{bulk} = k^{dry} + \sum_{\alpha=1}^{NP} \sqrt{S_\alpha} k_\alpha^{sat}.$$

The bulk conductivity can be set to a constant value by using the form
`(tcond` *<real-number>*`)`

*<KdFactor-parameters>*

Parameters for temperature dependent factor multiplying the solid sorption factor, $Kd$, for component *<comp>* (excluding `energy` component). Valid parameters are:
*<real>*

real number. Value of 1.0 means no temperature modification.

`KdFactorExp (fac1` *<fac1>*`) (T1` *<T1>*`) (T0` *<T0>*`)`

Units of temperatures *<T0>* and *<T1>* are in centigrade. The factor is unity at temperature *<T0>* and equal to *<fac1>* at temperature *<T1>*. At other values varies according to the formula

$$factor = \exp(-A/T_K)/\exp(-A/T_{K0})$$

Here $T_K$ is temperature in Kelvin and $T_{K0}$ is <*T0*> converted to Kelvin. The parameter $A$ is calculated from the model by the constraint that the factor equals <*fac1*> at <*T1*>.

**Component specific properties.**

```
(compprop

     (<comp>

          (intrinsic
               (MoleWt <molewt>)
               (solidHalfLife <solid-half-life>)      optional
          )

          (<phase>
               (freeDiffusivity <freeDiff>)
               (Keq <Keq-parameters>)
               (rhoC <rhoC-parameters>)          not used by gas phase
               (enthC <enthC-parameters>)        required only by thermal models
               (halfLife <fluid-half-life>)    optional
          )

          ...

          (<phase>
               ...
          )
     )

     ...

     (<comp>
          ...
     )

)
```

set component dependent properties.

*<phase>* *word*

Name of phase.

*<comp>* *real*

Name of component (excluding **energy** component).

*<molewt>* *real*

Molecular mass of the component (g/mole). (The model internally converts this value to kg/mole)

*<solid-half-life>* *real*
*<fluid-half-life>* *real*

Optional half life for first order decay for the component adsorbed on the solid phase and withing each of the fluid phases. The model internally calculates the decay constant $\lambda$ separately for each of the phases from the equation $\lambda = \ln(2)/\text{half} - \text{life}$ The ability to set the half-life separately for each phase is useful for bio or chemical degradation where decay may occur at different rates in each phase.

*<freeDiff>* *real*

Free molecular diffusion coefficient of the component within the specified phase ($m^2/s$).

*<Keq-parameters>*

Parameters specifying the equilibrium partitioning coefficient of a component. For a given component, a convenient reference phase should be chosen. The coefficient for reference phase is set to unity. All other coefficients are then defined with respect to the reference phase. That is, the coefficient for a component in phase, $\alpha$, is equal to the mole fraction of the component in the $\alpha$ phase divided by the mole fraction of the component in the reference phase. Thus, if the liquid phase is chosen as the reference phase, the coefficient for the gas phase is the ratio of the mole fraction in the gas to that of the mole fraction in the liquid. To prevent mathematical singularities, the coefficients should be set to nonzero positive numbers. A singularity will also result if there are two or more components which have the exactly the same coefficients. Valid options are:

*<real-number>*

Constant real number in mole/mole.

`KeqStd (A` *<A>*`) (B` *<B>*`) (C` *<C>*`) (D` *<D>*`)`

For isothermal,

$$Keq = A + pg * B + C/pg,$$

and for nonisothermal,

$$Keq = (A + pg * B + C/pg) * exp(-D/TKelv)$$

where $pg$ is gas pressure and $TKelv$ is temperature in Kelvin. The parameters *<A>*,*<B>*, and *<D>* are optional and default to zero. Assumes that the liquid phase is the reference phase.

`KeqTCESolute`

Coefficient for TCE in the gas phase. Assumes that the liquid phase is the reference phase.

`KeqWatVapor`

Coefficient for water vapor in the gas phase. Assumes that the liquid phase is the reference phase.

*<enthC-parameters>*

Parameters for calculating specific enthalpy of the component.
Valid options are:

*<real-number>*

Constant value (J/kg).

`enthCConstCp (Cp` *<Cp>*`) (Tref` *<Tref>*`) (Hv` *<Hv>*`)`

Calculate from formula

$$H = Cp * (T - Tref) + Hv$$

*<Cp>* Specific heat (J/kg-K).
*<Tref>* Reference temperature (degrees C).
*<Hv>* Reference enthalpy (J/kg).

`enthCConstCp (Cp` *<Cp>*`) (Tref` *<Tref>*`) (b` *<b>*`) (Tc` *<Tc>*`)`

Calculate from formula

$$H = Cp * (T - Tref) + a(T - T_c)^b$$

*<a>* Parameter.
*<b>* Parameter.
*<Tc>* Critical temperature (degrees C).

`enthCLiqWat`

Partial enthalpy of water component in pure aqueous phase (J/kg) calculated from steam tables. Can be used, as an approximation, for dilute solutions.

`enthCWatVap`

Partial enthalpy of water in pure water vapor phase (J/kg). Can be used, as an approximation, for water vapor in ideal gas mixtures.

*<rhoC-parameters>*

Parameters specifying the component partial mass density.
Valid options are:

`rhoCConstComp (p0` *<p0>*`)(rho0` *<rho0>*`)(compress <compress>)`

Formula based on constant compressiblity

$$\rho = \rho_0 \exp[c(p - p_0)]$$

Used for components in liquid phases.

| | |
|---|---|
| <*p0*> | Reference pressure $p_0$ (Pa). |
| <*rho0*> | Reference density $\rho_0$ (kg/m$^3$). |
| <*compress*> | Compressibility $c$ (1/Pa). |

`rhoCLiqWat`

Partial mass density of water for a pure liquid water phase calculated from steam tables (kg/m$^3$). Can be used, as an approximation for water component in a dilute aqueous phase.

**Phase specific properties.**

```
(phaseprop

    (<phase>
       (rhoP <rhoP-parameters>
       (viscosity <viscosity-parameters>
       (enthP <enthP-parameters>       only needed for thermal models
    )

    ...

    (<phase>
        ...
    )

)
```

set phase dependent properties.

*<phase>* *word*

Name of phase.

*<rhoP-parameters>*

Phase mass density.

`rhoPLinearMix`

Calculate phase density based on linear volumetric mixing rule

$$\frac{1}{\rho} = \sum_{\gamma} \frac{\omega^{\gamma}}{\rho^{\gamma}}$$

where $\omega^{\gamma}$ and $\rho^{\gamma}$ are the mass fractions and the partial mass density of the $\gamma$ component, respectively.

`rhoPZFacStm`

Phase density for the gas phase based on ideal gas law. If there is a component callde `water`, a "Z-factor" is used to correct for the water vapor density from steam tables.

`rhoPIdealGas`

Phase density for the gas phase based on ideal gas law.

`rhoPLiqWat`

Density of pure liquid water phase. Can be used as an approximation for a dilute aqueous phase.

*<viscosity-parameters>*

Parameters for dynamic viscosity.

*<real>*

Constant value (Nt-s/$m^2$).

`visLiqWat`

Viscosity of liquid water as function of pressure and temperature.

`visGasAirWat`

Viscosity of gas phase with air-water vapor mixture as function of pressure and temperature.

*<enthP-parameters>*

Specific enthalpy of the phase.

*<real>* constant value (J/kg).

`enthPLinearMix`

Use linear mixing of the component partial enthalpies.

**Generic properties.**

*used only for isothermal models*

```
(generic
     (T <T>)
)
```

*<T>* *real*

Initial temperature in centigrade. Ignored by thermal models. Initial temperature for thermal models are set by `state`.

**Read and write restart information.**

```
(read-restart
     (file "<file-name>")
     (time <restart-time>)    optional
)
```

"<*file-name*>" string

name of the restart file created by the option (output ...(restart ...) ...).

<*restart-time*> *real*

Time used to search in the restart file; the first restart record with time ¿= <*restart-time*> will be read in. The initial time of the simulation run is set by time and overwrites the time read in through the restart file. If time is not present, the initial of the run is set to the time read in.

**Overwriting Restart Data**

```
(overwrite-restart
     ...
)
```

The overwrite-restart statement is used to overwrite restart information read in from the read-restart statement for selected elements or variables. The overwrite-restart options are identical to those for the state statement.

**Restart Backup**

The model will periodically write out restart records so that the model can be restart in case of system failure. The model alternately writes out to two restart files named <*prefix*>.re0 and <*prefix*>.re1 where <*prefix*> is set by output-prefix. Each file contains a single record; previous records are overwritten. The reason for using two files instead of a single one is to prevent losing a record if the system fails during a write. The user must check the two files to see which has the record with the latest simulation time. The model writes to a file at periodic intervals based on the wall clock time.

(backup <*option*>) *optional*

<*option*> *word*

if set to on, then the model will periodically write backup restarts. If set to off, the model will not do backups. Default is on.

(backup-period <*backup-time*>) *optional*

<*backup-time*> t-real

wall clock time period for model to perform backup restarts. Default value is 10m (i.e., 10 minutes).

**Source terms.**

```
(srctab
     (compflux
          (comp <comp>)
          (name <compflux-name>)
          (range "<elem-range>" "<elem-range>" ...)
          (table  <comp-flux-table>)
          (enthalpy <enthalpy-table>)
     )
     ...
     (compflux
          ...
     )

     (phaseflux
          (phase <phase>)
          (name <phaseflux-name>)
          (range "<elem-range>" "<elem-range>" ...)
          (table  <phase-flux-table>)
          (setcomp-internal)
          (setcomp
               (<comp>
                    (table <conc-table>)
                          following only for thermal models
                    (enthalpy <enthalpy-table>)
               )
               ...
               (<comp>
                    ...
               )
          )
     )
     ...
     (phaseflux
          ...
     )

)
```

The parameters in `compflux` specifies a component mass flux (kg/s) into an element or range of elements through a table of source fluxes at specified points in time. Linear interpolation is used for time intervals between the table values. Positive flux is flux *into* an element; negative flux is *out* of an element. There may be several `compflux` sets.
The `phaseflux` parameters specifies a phase mass flux (kg/s) into an element or a range of elements through a table of source fluxes at specified points in time. Linear interpolation is used for time intervals between the table values. Positive flux is flux *into* an element; negative flux is *out* of an element. There may be several `phaseflux` sets. The user must specify the component concentrations withing the phase stream. An alternate option is to

use the internally model computed concentrations of each element.
Either `setcomp-internal` or setcomp options are used, but not both.
Important: One should use `(output ...(forcetimes ...))` (see NUFT User Manual) to force the model to hit specified times to prevent the model from skipping past at times when the flux table changes abruptly.

*<comp>* *name*

Name of component (includes `energy` component).

*<compflux-name>* *name*

Name of the component flux set. Used when referring to this set within output options.

"*<elem-range>*" *pattern string*

Source flux will be applied to those elements which matches any of the pattern strings. See NUFT User Manual for explanation of pattern strings.

*<comp-flux-table>* *list of reals*

Table of component mass fluxes of the form
*<t0> <q0> <t1> <q1> ...*
where the time values are given by *<t0>*, *<t1>*, ..., which are of data type *t-real* and the mass flux at these times are *<q0>*, *<q1>*, ..., which are of data type *real* and are in units of kg/sec. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run.

*<phase>* *name*

Name of the phase.

*<phaseflux-name>* *name*

Name of the phase flux set. Used when refering to this set within output options.

*<phase-flux-table>* *list of reals*

Table of mass fluxes of the phase that are of the form
*<t0> <q0> <t1> <q1> ...*
where the time values are given by *<t0>*, *<t1>*, ..., which are of data type *t-real* and the mass flux at these times are *<q0>*, *<q1>*, ..., which are of data type *real* and are in units of kg/sec. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run.

*<conc-table>* *list of reals*

Table of mole fraction concentrations of the components withing the phase stream. The table is of the form

*<t0> <x0> <t1> <x1> ...*

where the time values are given by *<t0>*, *<t1>*, ..., which are of data type *t-real* and the concentrations are *<x0>*, *<x1>*, ..., which are of data type *real*. An alternative is to specify the component concentrations used for the flux of applied to each respective element as that within the element itself, which is done by using the `setcomp-internal` command instead of `setcomp`.

*<enthalpy-table>* *list of reals*

Table of specific partial enthalpies of the component (J/kg). The table is of the form

*<t0> <h0> <t1> <h1> ...*

where the time values are given by *<t0>*, *<t1>*, ..., which are of data type *t-real* and the enthalpy at these times are *<h0>*, *<h1>*, ..., which are of data type *real* and have units of Joules/kg. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run.

`setcomp-internal`

Calculate component and energy fluxes based on concentrations and enthalphies in the respective phase within the element instead of specifying through a table of concentrations and enthalpies.

**Boundary conditions.**

```
(bctab

     (<bc-name>

          (basephase <phase>)

          (range "<elem-range>" "<elem-range>" ...)

          (tables
               (<variable> <var-table>)
               ...
               (<variable> <var-table>)
          )

                following is optional
          (factor
               (<comp> <factor-table>)
               ...
               (<comp> <factor-table>)
          )
     )

     ...

     (<bc-name>

          (basephase <phase>)

          (range "<elem-range>" "<elem-range>" ...)

          (clamped)

                following is optional
          (factor
               (<comp> <factor-table>)
               ...
               (<comp> <factor-table>)
          )
     )

     ...

     (<bc-name>
          ...
     )

)
```

Specifies boundary conditions. Boundary conditions are implemented by specifying values of the primary variables on special elements as functions of time.
Specification of primary variables at the boundary elements is the same as when specify-

ing initial conditions as in `state`. Thus, one uses negative concentrations as place holders for unneeded concentrations; however, unlike `state` no warning messages are printed if a concentration is set (i.e. non-negative) but is not necessary.
Important: One should use `(output ...(forcetimes ...))` (see NUFT User Manual) to force the model to hit specified times to prevent the model from skipping past at times when the variable or factor table changes abruptly.

"<*elem-range*>" *string pattern*

Those elements which matches any of the pattern strings will be elements which will be used to specify the boundary condition. See NUFT User Manual for explanation of pattern strings.

<*variable*> *word*

Primary variable (same as those in `state`).

<*var-table*>

Time dependent table of values of <*variable*> of the form
<*t0*> <*val0*> <*t1*> <*val1*> ...
where the time values are given by <*t0*>, <*t1*>, ..., which are of data type *t-real* and the values of the variables are <*val0*>, <*val1*>, ...are of data type *real*. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run.

<*comp*> *word*

Name of component in factor table (includes `energy` component). There must be a table for each component.

<*factor-table*>

Specify factor multiplying the component fluxes between the elements specified in `range` and other elements. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run. One use of this factor is to turn off or turn on fluxes at different times. The table is of the form
<*t0*> <*fac0*> <*t1*> <*fac1*> ...
where the time values are given by <*t0*>, <*t1*>, ..., which are of data type *t-real* and the factors at these times are <*fac0*>, <*fac1*>, ..., which are of data type *real*. Linear interpolation is used for values between the time values. The last time must be greater than the end time of the run.
Instead of applying a factor to component fluxes one can apply a factor to phase fluxes (see NUFT Reference Manual).

`(clamped)`

Keeps the primary variables for these elements, as set in `state`, fixed in time.

**Output options.**

Valid element output variables for the usnt module are:

| | |
|---|---|
| `P` | gas phase pressure (Pa). |
| `S.`<*phase*> | saturation of <*phase*>. |
| `C.`<*comp*>`.`<*phase*> | mole fraction of <*comp*> in <*phase*>. |
| `X.`<*comp*>`.`<*phase*> | mass fraction of <*comp*> in <*phase*>. |
| `T` | temperature (°C). |
| `Vmag.`<*phase*> | magnitude of pore velocity of a phase (m/s). |
| `Vel.`<*phase*> | $x$,$y$,$z$ components of the pore velocity (m/s), |
| valid only for `by-contour` option. `porosity` | porosity. |
| `vis.`<*phase*> | viscosity of a phase (Nt-s/m). |
| `Pc.`<*phase*> | capillary pressure of a phase (Pa). |
| `kr.`<*phase*> | relative permeability of a phase. |
| `Kx, Ky, Kz` | permeabilities ($m^2$/s) (see `genmsh` for definitions). |
| `log10Kx, log10Ky, log10Kz` | logarithm base 10 of permeabilities (log10 ($m^2$/s)) (see `genmsh` for de |
| `porosity` | porosity. |
| `Psat` | saturation pressure (valid only for nonisothermal option with water as one of the components). |
| `RH` | relative humidity w.r.t. an open system (valid only for nonisothermal option with water as one of the components). |

Valid connection output variables are:

| | |
|---|---|
| `V.`<*phase*> | pore velocity (m/s) in <*phase*>. |
| `q.`<*phase*> | specific mass flux of phase (kg/s-m$^2$). |
| `q.`<*comp*> | specific mass flux of component (kg/s-m$^2$) in all phases; if <*comp*> is 'energy', then output specific energy flux (W/m$^2$) in all phases including solid phase. |
| `q.`<*comp*>`.`<*phase*> | specific mass flux of component (kg/s-m$^2$) in <*phase*>; if <*comp*> is 'energy', then output specific energy flux (W/m$^2$) in <*phase*>. |
| `qd.`<*comp*> | specific diffusive mass flux of component (kg/s-m$^2$) in all phases; if <*comp*> is 'energy', then output specif diffusive energy flux (W/m$^2$) in all phases including solid. |
| `qd.`<*comp*>`.`<*phase*> | specific diffusive mass flux of component (kg/s-m$^2$) in <*phase*>; if <*comp*> is 'energy', then output specific diffusive energy flux (W/m$^2$) in <*phase*>. |
| `qa.`<*comp*> | specific advective mass flux of component (kg/s-m$^2$) in all phases; if <*comp*> is 'energy', then output specific diffusive energy flux (W/m$^2$) all phases includi |
| `qa.`<*comp*>`.`<*phase*> | specific advective mass flux of component (kg/s-m$^2$) in <*phase*>; if <*comp*> is 'energy', then output specific diffusive energy flux (W/m$^2$) in <*phase*> inclu |
| `qrad` | specific radiative thermal flux (W/m$^2$). |
| `qcond` | specific conducitive thermal flux (W/m$^2$). |
| `Q.`<*phase*> | total mass flux of phase (kg/s). |
| `Q.`<*comp*> | total mass flux of component (kg/s) in all phases; if <*comp*> is 'energy', then output total in all phases including solid. |
| `Q.`<*comp*>`.`<*phase*> | total mass flux of component (kg/s) in <*phase*>; if <*comp*> is 'energy', then output total energy flux (V |
| `Qd.`<*comp*> | total diffusive mass flux of component (kg/s) in all phases; if <*comp*> is 'energy', then output total diffusive energy flux (W) in all including solid. |
| `Qd.`<*comp*>`.`<*phase*> | total diffusive mass flux of component (kg/s) in <*phas* if <*comp*> is 'energy', then output total diffusive energ in <*phase*>. |
| `Qa.`<*comp*> | total advective mass flux of component (kg/s) in all phases; if <*comp*> is 'energy', then output total diffusive energy flux (W) in all phases including solid. |
| `Qa.`<*comp*>`.`<*phase*> | total advective mass flux of component (kg/s) in <*phase*>; if <*comp*> is 'energy', then output total diffusive energy flux (W) in <*phase*>. |
| `Qrad` | total radiative thermal flux (W). |
| `Qcond` | total conducitive thermal flux (W). |

```
(output

     (field
          (file-ext "<out-ext>")
          (format <options>)
          (index-range (<i0> <i1> <j0> <j1> <k0> <k1>)
                       ...
                       (<i0> <i1> <j0> <j1> <k0> <k1>)
          )
          (variables <el-var0> <el-var1> ...)
          (outtimes <t0> <t1> ...)
     )

     (flux-field
          (file-ext "<out-ext>")
          (format <options>)
          (index-crange
                ( (<i0> <j0> <k0>  <i1> <j1> <k1>)
                  ...
                  (<i0> <j0> <k0>  <i1> <j1> <k1>)
                )
          (variables <con-var0> <con-var1> ...)
          (outtimes <t0> <t1>  ...)
     )

     (history
          (file-ext "<out-ext>")
          (variable <el-var>)
          (element "<element-name>")
     )

     (flux-history
          (file-ext "<out-ext>")
          (variable <con-var>)
          (index-con <i0> <j0> <k0> <i1> <j1> <k1>)
     )

     (srcflux
          (comp <comp>)
          (file-ext "<out-ext>")
          (outtimes <t0> <t1> ...)
          (cumulative)    optional
     )

     (bcflux
          (comp <comp>)
          (file-ext "<out-ext>")
          (outtimes <t0> <t1> ...)
          (cumulative)    optional
     )

     (forcetimes
          (outtimes <t0> <t1> ...)
     )
```

```
     (restart
          (file-ext "<out-ext>")
          (outtimes <t0> <t1> ...)
     )

     (extool
          (file-ext "<out-ext>")
          (index-range (<i0> <i1> <j0> <j1> <k0> <k1>) ... )
          (variables <var0><var1> ...)
          (outtimes <t0> <t1> ...)
     )
)
```

specifies what variables will be dumped to files and the output format. Any of the above output options (`field`, `flux-field`, etc.) are optional or can be present any number of times in any order including with regards to different variables. (See below regarding other options and important notes.) Output options are:

| | |
|---|---|
| `field` | output variables of selected elements at specified times |
| `flux-field` | output fluxes between selected elements at specified times |
| `history` | output variables of selected elements at all times |
| `flux-history` | output the fluxes between selected elements at all times (not applicable to USNT model) |
| `srcflux` | output component fluxes for a flux specified in `srctab` |
| `bcflux` | output component fluxes flowing out of a set of boundary elements specified by `bctab` |
| `forcetimes` | force the model to hit the times specified in `outtimes` |
| `restart` | write out a restart record to a file that can be read in by `restart` option |
| `extool` | write out data in *extool* format. |

*<out-ext>* *string*

suffix of output file (`file-ext` is optional). The prefix of the output file name will be made up of the prefix set by the `output-prefix` parameter. (The suffix should be some mnemonic, e.g. the name of the variable being outputted.) For example, if `output-prefix` is set to "runA"and `file-ext` to ".C"then output will go to file "runA.C".
If the `file-ext` parameter is not present, then the output will be placed into the main output file. Output for different output options can share the same output file.

*<options>* *word*

format of output. Can be any of following:

| | |
|---|---|
| `list` or `by-list` | output values at elements along with the element names (contsac format |
| `by-set` | list element values as a vector of the form [#n v1 v2 ...vn] |
| `by-x` | list x coord. and value |
| `by-y` | list y coord. and value |
| `by-z` | list z coord. and value |
| `by-ijk` | list i,j,k index and value |
| `by-xtable` | format compatible with `state` using by-xtable method, user needs to comment out output header |
| `by-ytable` | format compatible with `state` using by-ytable method, user needs to comment out output header |

| | |
|---|---|
| `by-ztable` | format compatible with `state` using by-ztable method, user needs to comment out output header |
| `tabular` | multi-column format |
| `contour` | format readable by the `nview` program for MS-DOS |

*<index-range>* list of *integers*

range of elements specified by the $i, j, k$ indices.

*<comp>* *word*

component name.

*<el-var>* *word*
*<el-var0>*, *<el-var1>* list of *words*

list of element variables that will be outputted (model specific).

*<con-var>* *word*
*<con-var0>*, *<el-var1>* list of *words*

list of connection variables (e.g. fluxes) that will be outputted (model specific).

*<outtimes>* list of *t-reals*

list of times at which output will be performed. Model will reduce the time steps to meet these times.

*<index-crange>* list of lists of *integers*

specifies a list of connections. Comprised of a list of list of integers with each list specifying a connection. Each list of integers is of the form

(*<i0> <j0> <k0> <i1> <j1> <k1>*)

and denotes the connection between element $i$ =*<i0>*, $j$ =*<j0>*, $k$ =*<k0>* and element $i$ =*<i1>*, $j$ =*<j1>*, $k$ =*<k1>*. Positive flux denotes flux from the first element to the second.

*<out-var-name>* *word*

name of output variable to be outputted by `history` option (model specific).

"*<element-name>*" *string*

name of element whose state, or primary, variable will be outputted.

*<index-con>* list of *integers*

specifies the single connection between the element ($i$ =*<i0>*, $j$ =*<j0>*, $k$ =*<k0>*) and the element ($i$ =*<i1>*, $j$ =*<j1>*, $k$ =*<k1>*). Positive flux denotes flux flowing from the first element to the second.

*<bc-name>* *word*

name of boundary condition used in `bctab`.

*<src-name>* *word*

name of source term used in `srctab`.

`(cumulative)`

optional. If present, the cumulative flux is outputted. If not present, the instantaneous flux is outputted. Note that cumulative fluxes are reset to zero at the beginning of a restart.

**Notes:**

1. Instead of `(file-ext "`*<out-ext>*`")` one can use `(file "`*<file-name>*`")` in order to explicitly specify the output file.
2. `(outtimes` *<t0> <t1> <t2>* ...`)` can be replaced by either of:

   a. `(outtimes *)` which means all times.

   b.

   ```
   (triggers
       ((wake <state-var> (range "<el-name>"  "<el-name>" ...)  <op> <val>)
        (cond <state-var> (range "<el-name>"  "<el-name>" ...)  <op> <val>)
       )
       ...
       ((wake <state-var> (range "<el-name>"  "<el-name>" ...)  <op> <val>)
        (cond <state-var> (range "<el-name>"  "<el-name>" ...)  <op> <val>)
        )
   )
   ```

   which checks to see at every time step if any of the triggers goes off. A trigger goes off iff its wake condition *<value> <op> <val>* is true where *<value>* is the value of the state variable *<state-var>* at the elements with names in the range of any of the pattern strings "*<el-name>*" .... If the wake condition is true, then the condition in the `cond` field is checked; if true then the trigger goes off and output occurs. Triggers can go off only once.
3. One can use `(range "`*<element-range>*`"...)` instead of `index-range` to specify elements by the names where "*<element-range>*" is a *pattern string*.
4. Similarly, one can use `(crange ("`*<element-range-0>*`" "`*<element-range-2>*`") ...)` instead of `(index-crange ((`*<i0> <j0> <k0> <i1> <j1> <k1>*`) ...))` to specify ranges of elements. Here, `("`*<element-range-0>*`" "`*<element-range-1>*`")` specifies all possible connections between elements whose names match the pattern string "*<element-range-0>*" and the elements whose names match "*<element-range-1>*".
5. One can use `(connection "`*<element-name-0>*`" "`*<element-name-1>*`")` instead of `(index-con` *<i0> <j0> <k0> <i1> <j1> <k1>*`)` to specify a connection.

**Vapor pressure lowering option.**

the model implements vapor pressure lowering. the default is on. to turn off vapor pressure lowering add the following to the topmost input level:

```
(vapor-pressure-lowering off)
```

### 6.1. Notes: Table Time Values

Currently, the model may in some cases choose time steps which are so large that it overshoots sharp changes in a time table. This may be a serious problem if, for example, we want to model a flux that is turned off suddenly. A solution is to use the `forcetimes` command in `output` which forces the model to hit specified times, in this case, the times at which the boundary condition changes suddenly.

The last time value in table must be greater than or equal to the ending time of the simulation as set by `tstop` or the model will abort.

## 7. References

Lee, K., A. Kulshrestha, and J. Nitao, Interim Report on Verification and Benchmark Testing of the NUFT Computer Code, Lawrence Livermore National Laboratory Report UCRL-ID-113521, 1993.

Nitao, J.J., Reference manual for the NUFT flow and transport code, Lawrence Livermore National Laboratory Report, UCRL-ID-113520, 1995.

## A. Sample Problem No. 1: Isothermal

**Description:**

Two-dimensional isothermal infiltration problem in a cylindrically symmetric system with "point" constant head source of water. Three soil types. The source is turned off after 200 minutes. A conservative tracer is introduced along with the water.

**Input file:**

```
;;;file: usnsam1.in;;;
;; sample problem
(usnt  ;; name of flow model
     (modelname flow)
     (title "usnt sample #1")       ;; run title
     (tstop 23.1h)            ;; stopping time is 23.1 hours
     (stepmax 1000)           ;; maximum no. of time steps
     (time 0.0)               ;; initial time
     (dtmax 1.e30)            ;; maximum time step
     (dt 1m )                 ;; initial time step is 1 minute

     (init-eqts
          (components water air contam)
          (phases liquid gas)
          (primary-phase gas)
          (wetting-phase liquid)
          (isothermal)
     )

     (input-mass-fraction off)  ;; use mole fraction C instead of mass fraction

     ;;;; uncomment following lines for preconditioned conjugate gradient
     ;;;; method:
     ;;     (linear-solver pcg)
     ;;     (pcg-parameters  (precond d4) (north 15) (toler 1.e-5)
     ;;                      (itermax 100))
     ;;     (ilu-degree 1)

     ;; set output formats
     (output
          ;; outputs all liquid saturation into file "usnsam1.Sl"
          (field (format list) (range "*") (variables S.liquid)(file-ext ".Sl")
                 (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
          )
          ;; outputs aqueous phase concentration of contaminant
          ;; into file "usntsam1.Con"
          (field (format list) (range "*")
                 (variables C.contam.liquid)
                 (file-ext ".Con")
                 (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
          )
          ;; outputs all pressure into file "usntsam1.P"
          (field (format list) (range "*") (variables P)(file-ext ".P")
                 (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
```

```
      )
      ;; output liquid phase flux from source into file "usntsam1.inf"
      (bcflux (comp water) (name src) (file-ext ".inf")
            (outtimes *))

      ;; force model to hit specific times when source is shut off
      (forcetimes (outtimes 200m 201m)
      )
) ;; end output

;; set material properties
(rocktab
      ;; sandy material
      (HI
            (porosity  0.25)
            (Kd
               (contam 0.0)  ;; conservative tracer
               (air 0.0)
               (water 0.0))
            (Kx 1.53e-12)(Ky 0.)(Kz 0.)
            (pc (liquid  pcVanGen (m 0.6)(alpha 5.1e-4)(Sj 0.41)(Sr 0.4)))
            (kr (gas krgVanGen (m  0.6)(Sr 0.05))
                (liquid krlVanGen (m  0.6)(Sr 0.4)))
            (tort (liquid Millington (Sr 0.4)) (gas Millington (Sr 0.05)))
      )
      ;; moderate permeability material
      (MOD   (porosity  0.3)
            (Kd
               (contam 0.0)  ;; conservative tracer
               (air 0.0)
               (water 0.0))
            (Kx 1.53e-13)(Ky 0.)(Kz 0.)
            (pc (liquid pcVanGen (m 0.3)(alpha 1.0e-4)(Sj  0.41)(Sr 0.4)))
            (kr (gas krgVanGen (m  0.3)(Sr 0.05))
                (liquid krlVanGen (m  0.3)(Sr 0.4)))
            (tort (liquid Millington (Sr 0.4))(gas Millington (Sr 0.05)))
      )
      ;; clayey material
      (LO    (porosity  0.3)
            (Kd
               (contam 0.0)  ;; conservative tracer
               (air 0.0)
               (water 0.0))
            (Kx 1.5e-14)(Ky 0.)(Kz 0.)
            (pc (liquid   pcVanGen (m 0.2)(alpha 5.1e-5)(Sj  0.41)
                        (Sr 0.4)))
            (kr (gas krgVanGen (m  0.2)(Sr 0.05))
                (liquid krlVanGen (m  0.2)(Sr 0.4)))
            (tort (liquid Millington (Sr 0.4))(gas Millington (Sr 0.05)))
      )
     ;; pseudo soil type for source element above surface
     (SRC   (porosity  0.99)
            (Kd
               (contam 0.0)  ;; conservative tracer
```

```
                (air 0.0)
                (water 0.0))
             (Kx 1.e-9)(Ky 0.)(Kz 0.)
             (pc (liquid   0.0))  ;; zero cap. pressure
             (kr (gas 0.0)(liquid 1.0))  ;; gas rel. perm. set to zero
                                         ;; liquid rel. perm. set to unity
             (tort (liquid 0.0)(gas 0.0)) ;; turn off all diffusive fluxes
      )
      ;; pseudo soil type for inactive elements (no. perm.) above surface
      (INACT (porosity  0.99)
             (Kd
                (contam 0.0)  ;; conservative tracer
                (air 0.0)
                (water 0.0))
             (Kx 0.)(Ky 0.)(Kz 0.)
             (pc (liquid   0.0))
             (kr (gas 0.0)(liquid 0.0))
             (tort (liquid 0.0)(gas 0.0))
      )

   ) ;; end rocktab

   ;; phase properties
   (phaseprop
      (liquid
         (rhoP rhoPLiqWat)
         (viscosity visLiqWat)
      )
      (gas
         (rhoP rhoPZFacStm)
         (viscosity visGasAirWat)
      )
    ) ;; end phaseprop

   ;; component properties
   (compprop
      (water
            (intrinsic (MoleWt 18.))
            (gas    (Keq KeqWatVapor)
                    (freeDiffusivity 1.e-4))
            (liquid (freeDiffusivity 1.e-9)
                    (Keq 1.0)
                    (rhoC rhoCLiqWat))
       )
      (air
            (intrinsic (MoleWt 29.))
            (gas    (Keq KeqStd (C 0.973e11)(D 0.0))
                    (freeDiffusivity 1.e-4))
            (liquid (freeDiffusivity 1.e-9)
                    (Keq 1.0))
      )

      (contam  ;; contaminant
            (intrinsic (MoleWt 130.))
```

```
            (gas    (Keq KeqTCESolute)
                    (freeDiffusivity 1.e-4))
            (liquid (freeDiffusivity 1.e-9)  (Keq 1.0)
                    (rhoC rhoCLiqWat))
      )
   );;end component properties

(generic
       (T 15.)     ;; temperature in degrees C
 )

;; set boundary conditions
(bctab
     ;; put flux into the source element
     (src
          (range "S*")
          (basephase liquid)
          ;; turn source on from 0 to 200 min. and off after that
          (factor  (water  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
                   (contam  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
                   (air  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
          )
          ;; set element to constant head of 3.5 meters
          (tables
                  (S.liquid  0. 1.0  1.e30 1.0)
                  (P   0.  1.34e5 1.e30  1.34e5)
                  (C.contam   0.  0.001 1.e30 0.001)
                  (C.air  0. 1.e-6 1.e30 1.e-6)
          )
     )

     ;; keep water table elements at saturated conditions
     (WT
          (range "W*")
          (basephase liquid)
          (tables
                  (S.liquid  0. 0.95  1.e30 0.95)
                  (P   0.  1.e5 1.e30  1.e5)
                  (C.contam   0.  0.0 1.e30 0.0)
                  (C.air  0. 1.e-6 1.e30 1.e-6)
          )
     )
 )  ;; end bctab

;; initial conditions
(state
     (S.liquid
         by-key ("S*" 1.0 ) ("I*" 1.0) ("H*" 0.2) ("M*" 0.3) ("L*" 0.8)
                ("W*" 0.95)
     )
     (C.contam  by-key ("*" 0.0))
     (C.air
         by-key ("S*" 1.e-6) ("I*" 1.e-6) ("H*" -1.) ("M*" -1.)
                ("L*" -1.)   ("W*" 1.e-6)
```

```
        )
        (P  by-key   ("*"    1.e5))  ;; note that bctab will overwrite
                                     ;; these values by any set there
    ) ;; end state

    ;; generate mesh
    (genmsh
       (coord cylind)
       ;; note that increasing z coordinate will be downward
       (down 0. 0. 1.)

       ;; set subdivisions in radial r direction
       (dx
              0.05  ;; 0.05 radius source
              0.1   ;; r = 0.15
              0.2   ;; r = 0.35
              0.4   ;; r = 0.75
              0.5   ;; r = 1.25
              0.5
              0.5
              0.5   ;; note: nr = 8
       )

       ;; set angle subdivision
       (dy 360.)

       ;; set subdivisions in z direction
       (dz
              0.01  ;; set first row of elements which are inactive
                    ;; except for i=1 for surface flux
               1.0   ;; sandy material layer
               1.0   ;; moderate material layer
               1.0   ;; sandy material layer
               1.0   ;; clay material layer
               1.0   ;; sandy material layer
               0.01  ;; water table k=7
       )

       ;; set material type and element name prefix
       (mat
               (S SRC   1 1  1 1  1 1)    ;; source element
               (I INACT 2 8  1 1  1 1)    ;; inactive elements
               (H HI    1 8  1 1  2 2)    ;; sandy layer
               (M MOD   1 8  1 1  3 3)    ;; moderate perm
               (H HI    1 8  1 1  4 4)    ;; sandy
               (L LO    1 8  1 1  5 5)    ;; clay
               (H HI    1 8  1 1  6 6)    ;; sandy
               (W HI    1 8  1 1  7 7)    ;; water table elements
       )
    ) ;; end genmsh

) ;;; end of input
```

## B. Sample Problem No. 2: Thermal

**Description:**

Same problem as Problem No. 1 but non-isothermal. The ground condition is kept fixed at 25 degrees C while the subsurface is initialized at 15 degrees C. The saturated zone at the bottom of the model is kept fixed at 15 degrees C. Another difference is that the topmost elements are no longer inactive elements but are modified to serve to simulate fixed atmospheric conditions.

**Input file:**

```
;; file: usnsam2.in;;;
;; sample problem
(usnt  ;; name of flow model
     (modelname flow)
     (title "usnt sample #2")       ;; run title
     (tstop 23.1h)            ;; stopping time is 23.1 hours
     (stepmax 1000)           ;; maximum no. of time steps
     (time 0.0)               ;; initial time
     (dtmax 1.e30)            ;; maximum time step
     (dt 1m )                 ;; initial time step is 1 minute

     ;; absolute time step tolerance
     (tolerdt (P 1.e5)(S 0.25)(C 0.1)(C.contam 1.e-4)(T 15.0))
     ;; relative time step tolerance
     (reltolerdt (P 0.2)(S 0.0)(C 0.1)(T 0.1))
     ;; absolute NR conv. tolerance
     (tolerconv (P 100.)(S 1.e-3)(C 1.e-3)(C.contam 1.e-5)(T 0.001))
     ;; absolute NR conv. tolerance
     (reltolerconv (P 1.e-3)(S 0.0)(C 1.e-4)(T 1.e-4))

     (init-eqts
          (components water air contam)
          (phases liquid gas)
          (primary-phase gas)
          (wetting-phase liquid)
          (thermal)
     )

     (input-mass-fraction off)  ;; use mole fraction C instead of mass fraction

     ;;;; uncomment following lines for preconditioned conjugate gradient
     ;;;; method:
     ;;     (linear-solver pcg)
     ;;     (pcg-parameters  (precond d4) (north 15) (toler 1.e-5)
     ;;                      (itermax 100))
     ;;     (ilu-degree 1)

     ;; set output formats
     (output
          ;; outputs all liquid saturation into file "usnsam2.Sl"
          (field (format list) (range "*") (variables S.liquid)(file-ext ".Sl")
                 (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
          )
```

```
        ;; outputs temperature into file "usnsam2.T"
        (field (format list) (range "*") (variables T)(file-ext ".T")
               (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
        )
        ;; outputs aqueous phase concentration of contaminant
        ;; into file "usnsam2.Con"
        (field (format list) (range "*")
               (variables C.contam.liquid)
               (file-ext ".Con")
               (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
        )
        ;; outputs all pressure into file "usnsam2.P"
        (field (format list) (range "*") (variables P)(file-ext ".P")
               (outtimes 0 39m 70m 102m 222m 287m 342m 23h)
        )
        ;; output liquid phase flux from source into file "usnsam2.inf"
        (bcflux (comp water) (name src) (file-ext ".inf")
               (outtimes *))

        ;; force model to hit specific times when source is shut off
        (forcetimes (outtimes 200m 201m)
        )
    ) ;; end output

    ;; set material properties
    (rocktab
        ;; sandy material
        (HI    (porosity  0.25)
               (Kd
                  (contam 0.0)  ;; conservative tracer
                  (air 0.0)
                  (water 0.0))
               (KdFactor (water 1.0)(air 1.0)(contam 1.0))
               (Cp 840)(solid-density 2580)
               (tcond tcondSqrt (solid 1.74)(liquid 2.34)(gas 1.74))
               (Kx 1.53e-12)(Ky 0.)(Kz 0.)
               (pc (liquid  pcVanGen (m 0.6)(alpha 5.1e-4)(Sj 0.41)
                   (Sr 0.4)))
               (kr (gas krgVanGen (m  0.6)(Sr 0.05))
                   (liquid krlVanGen (m  0.6)(Sr 0.4)))
               (tort (liquid Millington (Sr 0.4))
                     (gas Millington (Sr 0.05)))
        )
        ;; moderate permeability material
        (MOD   (porosity  0.3)
               (Kd
                  (contam 0.0)  ;; conservative tracer
                  (air 0.0)
                  (water 0.0))
               (KdFactor (water 1.0)(air 1.0)(contam 1.0))
               (Cp 840)(solid-density 2580)
               (tcond tcondSqrt (solid 1.74)(liquid 2.34)(gas 1.74))
               (Kx 1.53e-13)(Ky 0.)(Kz 0.)
               (pc (liquid pcVanGen (m 0.3)(alpha 1.0e-4)(Sj  0.41)
```

```
            (Sr 0.4)))
        (kr (gas krgVanGen (m  0.3)(Sr 0.05))
            (liquid krlVanGen (m  0.3)(Sr 0.4)))
        (tort  (liquid Millington (Sr 0.4))
               (gas Millington (Sr 0.05)))
 )
 ;; clayey material
 (LO    (porosity  0.3)
        (Kd
           (contam 0.0)  ;; conservative tracer
           (air 0.0)
           (water 0.0))
        (KdFactor (water 1.0)(air 1.0)(contam 1.0))
        (Cp 840)(solid-density 2580)
        (tcond tcondSqrt (solid 1.74)(liquid 2.34)(gas 1.74))
        (Kx 1.5e-14)(Ky 0.)(Kz 0.)
        (pc (liquid   pcVanGen (m 0.2)(alpha 5.1e-5)(Sj  0.41)
            (Sr 0.4)))
        (kr (gas krgVanGen (m  0.2)(Sr 0.05))
            (liquid krlVanGen (m  0.2)(Sr 0.4)))
        (tort (liquid Millington (Sr 0.4))
              (gas Millington (Sr 0.05)))
 )
;; pseudo soil type for source element above surface
(SRC   (porosity  0.99)
        (Kd
           (contam 0.0)  ;; conservative tracer
           (air 0.0)
           (water 0.0))
        (KdFactor (water 1.0)(air 1.0)(contam 1.0))
        (Cp 840)(solid-density 2580)
        (tcond tcondSqrt (solid 1.74)(liquid 2.34)(gas 1.74))
        (Kx 1.e-9)(Ky 0.)(Kz 0.)
        (pc (liquid   0.0))  ;; zero cap. pressure
        (kr (gas 0.0)     ;; gas rel. perm. set to zero
            (liquid 1.0)) ;; liquid rel. perm. set to unity
        (tort (liquid 0.0);; turn off all diffusive fluxes
              (gas 0.0))
 )
 ;; pseudo soil type for atmosphere above ground surface
 (ATM (porosity  0.99)
        (Kd
           (contam 0.0)  ;; conservative tracer
           (air 0.0)
           (water 0.0))
        (KdFactor (water 1.0)(air 1.0)(contam 1.0))
        (Cp 840)(solid-density 2580)
        (tcond tcondSqrt (solid 1.74)(liquid 2.34)(gas 1.74))
        (Kx 0.)(Ky 0.)(Kz 0.)
        (pc (liquid   0.0))
        (kr (gas krLinear (Sr 0.0)) (liquid 1.0))
        (tort (liquid 0.0) (gas 1.0))
 )
```

```
) ;; end rocktab

;; phase properties
(phaseprop
     (liquid
        (rhoP rhoPLiqWat)
        (viscosity visLiqWat)
        (enthP enthPLinearMix)
        (pcTemFac watPcTemFac)
     )
     (gas
        (rhoP rhoPZFacStm)
        (viscosity visGasAirWat)
        (enthP enthPLinearMix)
     )
 ) ;; end phaseprop

;; component properties
(compprop
     (water
           (intrinsic (MoleWt 18.))
           (gas
                   (Keq KeqWatVapor)
                   (freeDiffusivity 1.e-4)
                   (enthC enthCWatVap))
           (liquid (freeDiffusivity 1.e-9) (Keq 1.0)
                   (enthC enthCLiqWat)
                   (rhoC rhoCLiqWat))
      )
     (air
           (intrinsic (MoleWt 29.))
           (gas (Keq KeqStd (C 0.973e11)(D 0.0))
                   (freeDiffusivity 1.e-4)
                   (enthC enthCConstCp (Cp 1009.0)(Tref 0.0) (Hv 0.0)) )
           (liquid (freeDiffusivity 1.e-9)   (Keq 1.0) (enthC 0.0)  )
     )

     (contam  ;; contaminant
           (intrinsic (MoleWt 130.))
           (gas
                   (Keq KeqTCESolute)
                   (freeDiffusivity 1.e-4) (enthC 0.0))
           (liquid (freeDiffusivity 1.e-9)  (Keq 1.0)
                   (rhoC rhoCLiqWat)
                   (enthC 0.0))
      )
);;end component properties

;; set boundary conditions
(bctab
     ;; put flux into the source element
     (src
          (range "S*")
          (basephase liquid)
```

```
            ;; turn source on from 0 to 200 min. and off after that
            (factor  (water  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
                     (contam  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
                     (air  0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
                     (energy 0.0 1.0  200m 1.0 201m 0.0 1.e30 0.0)
            )
            ;; set element to constant head of 3.5 meters
            (tables
                    (S.liquid  0. 1.0  1.e30 1.0)
                    (P   0.  1.34e5 1.e30  1.34e5)
                    (C.contam   0.  0.001 1.e30 0.001)
                    (C.air  0. 1.e-6 1.e30 1.e-6)
                    (T 0. 15. 1.e30 15.)
            )
       )

       ;; keep water table elements at saturated conditions
       (WT
            (range "W*")
            (basephase liquid)
            ;; instead of tables we could have used (clamped) option
            (tables
                    (S.liquid  0. 1.0  1.e30 1.0)
                    (P   0.  1.e5 1.e30  1.e5)
                    (C.contam   0.  0.0 1.e30 0.0)
                    (C.air  0. 1.e-6 1.e30 1.e-6)
                    (T 0. 15. 1.e30 15.)
            )
       )

       ;; fix conditions at atmosphere elements
       (atmos (range "A*") (clamped))

    )  ;; end bctab

  ;; initial conditions
  (state
       (S.liquid
           by-key ("S*" 1.0 ) ("A*" 0.0) ("H*" 0.2) ("M*" 0.3) ("L*" 0.8)
                  ("W*" 1.0)
       )
       (C.contam  by-key ("*" 0.0))
       (C.air
           by-key ("S*" 1.e-6) ("A*" 0.99) ("H*" -1.) ("M*" -1.)
                  ("L*" -1.)   ("W*" 1.e-6)
       )
       (P  by-key   ("*"    1.e5))  ;; note that bctab will overwrite
                                    ;; these values by any set there
       (T by-key ("*" 15.)("A*" 25.))
  ) ;; end state

  ;; generate mesh
  (genmsh
     (coord cylind)
```

```
        ;; note that increasing z coordinate will be downward
        (down 0. 0. 1.)

        ;; set subdivisions in radial r direction
        (dx
               0.05  ;; 0.05 radius source
               0.1   ;; r = 0.15
               0.2   ;; r = 0.35
               0.4   ;; r = 0.75
               0.5   ;; r = 1.25
               0.5
               0.5
               0.5   ;; note: nr = 8
        )

        ;; set angle subdivision
        (dy 360.)

        ;; set subdivisions in z direction
        (dz
               0.01  ;; set first row of elements which are inactive
                     ;; except for i=1 for surface flux
                1.0   ;; sandy material layer
                1.0   ;; moderate material layer
                1.0   ;; sandy material layer
                1.0   ;; clay material layer
                1.0   ;; sandy material layer
                0.01  ;; water table k=7
        )

        ;; set material type and element name prefix
        (mat
                (S SRC   1 1  1 1  1 1)    ;; source element
                (A ATM   2 8  1 1  1 1)    ;; atmosphere elements
                (H HI    1 8  1 1  2 2)    ;; sandy layer
                (M MOD   1 8  1 1  3 3)    ;; moderate perm
                (H HI    1 8  1 1  4 4)    ;; sandy
                (L LO    1 8  1 1  5 5)    ;; clay
                (H HI    1 8  1 1  6 6)    ;; sandy
                (W HI    1 8  1 1  7 7)    ;; water table elements
        )
    ) ;; end genmsh

) ;;; end of input
```

## C. The Mathematical Model

We give the balance equations solved by the USNT model. Suppose we have NC number of components and NP number of phases. The solid phase is assumed nondeformable. The mass balance equations for the $\gamma = 1, \ldots, NC$ components are

$$\frac{\partial}{\partial t} \sum_{\alpha} \phi \rho_{\alpha} S_{\alpha} \omega_{\alpha}^{\gamma} = - \sum_{\alpha} \nabla \cdot \phi \rho_{\alpha} S_{\alpha} (\omega_{\alpha}^{\gamma} \mathbf{V}_{\alpha} + \mathbf{J}_{h\alpha}^{\gamma} + \mathbf{J}_{\alpha}^{*\gamma_{\alpha}}) - \sum_{\alpha} \lambda_{\alpha}^{\gamma} \phi \rho_{\alpha} S_{\alpha} \omega_{\alpha}^{\gamma} \tag{1}$$

where Fickian laws for dispersive and diffusive fluxes are given by

$$\mathbf{J}_{h\alpha}^{\gamma} = -\boldsymbol{D}_{h\alpha}^{\gamma} \nabla \omega_{\alpha}^{\gamma} \tag{2}$$

$$\mathbf{J}_{\alpha}^{*\gamma} = -D_{\alpha}^{*\gamma} \nabla \omega_{\alpha}^{\gamma} \tag{3}$$

and Darcy's law gives

$$S_{\alpha} \phi \mathbf{V}_{\alpha} = -\frac{\boldsymbol{k}_{\alpha}(S_{\alpha})}{\mu_{\alpha}} \cdot (\nabla p_{\alpha} + \rho_{\alpha} g \nabla z) \tag{4}$$

The retention pressure ("capillary pressure") relationships are given by

$$p_{\alpha} = p_g - p_{c\alpha}(S_{\delta}), \qquad \alpha \neq g. \tag{5}$$

The various variables are defined as

| | |
|---|---|
| $\omega_{\alpha}^{\gamma}$ | mass fraction of $\gamma$-component in phase $\alpha$ |
| $S_{\alpha}$ | liquid saturation of $\alpha$-phase |
| $\phi$ | porosity |
| $\rho_{\alpha}$ | mass phase density |
| $\omega_{\alpha}^{\gamma}$ | mass fraction |
| $\lambda_{\alpha}^{\gamma}$ | decay constant ( $= \ln(2)/\text{half} - \text{life}$ |
| $\mathbf{V}_{\alpha}$ | liquid phase velocity |
| $\mathbf{J}_{h\alpha}^{\gamma}$ | hydrodynamic dispersive flux |
| $\mathbf{J}_{\alpha}^{*\gamma}$ | molecular diffusive flux |
| $\boldsymbol{D}_{h\alpha}$ | dispersion tensor |
| $D_{\alpha}^{*\gamma}$ | diffusion coefficient |
| $\boldsymbol{k}_{\alpha}$ | permeability function |
| $\mu_{\alpha}$ | liquid phase viscosity |
| $p_{\alpha}$ | phase pressure |
| $p_{c\alpha}$ | retention pressure function |

The hydrodynamic dispersion flux, $\mathbf{J}_{h\alpha}^{\gamma}$, is not currently implemented in the model. In addition to the balance equations we have the constraints

$$\sum_{\gamma} \omega_{\alpha}^{\gamma} = 1 \tag{6}$$

$$\sum_{\alpha} S_{\alpha} = 1. \tag{7}$$

The model assumes local thermodynamic equilibrium and partitioning of components between phases are expressed in terms of partitioning coefficients,

$$n_{\alpha}^{\gamma} = \mathcal{K}_{\alpha,\beta}^{\gamma} n_{\beta}^{\gamma}. \tag{8}$$

where $\mathcal{K}_{\alpha,\beta}$ is a function of pressure and temperature. The variables $n_{\alpha}^{\gamma}$ and $n_{\beta}^{\gamma}$ are the mole fractions of the $\gamma$-component in the $\alpha$ and $\beta$ phases. They are related to the mass fractions by

$$n_{\alpha}^{\gamma} = (\omega_{\alpha}^{\gamma}/M^{\gamma}) \Big/ \left( \sum_{(\lambda)} \omega_{\alpha}^{\lambda}/M^{\lambda} \right). \tag{9}$$

The balance equation for energy is

$$\frac{\partial}{\partial t}\left[\sum_{\alpha}\phi\rho_{\alpha}u_{\alpha}S_{\alpha}+(1-\phi)\rho_{s}C_{p}(T-T_{ref})\right]= \sum_{\gamma}\sum_{\alpha}\left[\nabla\cdot\phi h_{\alpha}^{\gamma}\rho_{\alpha}S_{\alpha}(\omega_{\alpha}^{\gamma}\mathbf{V}_{\alpha}+\mathbf{J}_{h\alpha}^{\gamma}+\mathbf{J}_{\alpha}^{*\gamma_{\alpha}})\right]+\nabla\cdot K_{H}\nabla T \tag{10}$$

where

| | |
|---|---|
| $T$ | temperature |
| $C_p$ | specific heat of solid |
| $\rho_s$ | solid density |
| $u_\alpha$ | specific internal energy |
| $h_\alpha^\gamma$ | partial specific enthalpy |
| $K_H$ | thermal conductivity. |

Mixing laws are used to compute phase quantities from component quantities. Currently available ones are as follows

$$\frac{1}{\rho_{\alpha}}=\sum_{\gamma}\frac{\omega_{\alpha}^{\gamma}}{\rho_{\alpha}^{\gamma}} \tag{11}$$

$$h_{\alpha}=\sum_{\gamma}\omega_{\alpha}^{\gamma}h_{\alpha}^{\gamma} \tag{12}$$

Currently, phase viscosities correlation are available for pure water in the liquid phase and water-air mixture for the gas phase. Constant phase viscosity values may also be used. Future plans include various mixing laws and viscosity correlations.

The balance equations are discretized in space using the integrated finite difference method, and discretized in time using the fully implicity backward Euler method. The resulting nonlinear system of NC+1 equations are solved at each time step using the Newton Raphson method (see NUFT Reference Manual).